WHAT IS CLAIMED IS:

1. A computer-implemented process for automatically identifying compounds in a sample mixture, the process comprising:

receiving a representation of a measured condition of the sample mixture;

using said representation of a measured condition of the sample mixture to select a set of reference spectra of compounds suspected to be contained in said sample mixture, from a library of reference spectra;

receiving a representation of a test spectrum having peaks associated with compounds therein, said test spectrum being produced from the sample mixture under said measured condition; and

combining reference spectra from said set of reference spectra to produce a matching composite spectrum having peaks associated with at least some of said suspected compounds, that match peaks in said test spectrum, the compounds associated with the reference spectra that combine to produce the matching spectrum being indicative of the compounds in the sample mixture.

2. The process of claim 1 further comprising identifying compounds associated with said representative reference spectra.

3. The process of claim 2 wherein identifying compounds comprises identifying quantities of said compounds.

4. The process of claim 2 wherein identifying compounds comprises identifying concentrations of said compounds.

5. The process of claim 1 further comprising identifying a peak associated with a calibration compound, in said test spectrum.

6. The process of claim 5 wherein identifying a peak comprises identifying a peak meeting a set of criteria that associate said peak with said calibration compound.

7. The process of claim 5 wherein identifying comprises producing Lorentzian line shape parameters to represent said peak.

8. The process of claim 1 further comprising receiving a measured condition value representing a measured condition of the sample.

9. The process of claim 8 further comprising producing said measured condition value.

10. The process of claim 9 wherein producing said measured condition value comprises measuring pH of the sample.

11. The process of claim 9 wherein producing said condition value comprises producing said condition value from said test spectrum.

12. The process of claim 11 wherein producing said condition value comprises identifying in said test spectrum a peak position associated with a condition reference compound.

13. The process of claim 12 wherein identifying a peak position comprises identifying a peak meeting a set of criteria that associate said peak with said condition reference compound.

14. The process of claim 12 wherein producing said condition value comprises producing said condition value as a function of said peak position and parameters of a sample solvent.

15. The process of claim 9 wherein producing said condition value comprises determining a pH value for the sample, from said test spectrum.

16. The process of claim 15 wherein determining a measured pH value comprises determining from said test spectrum, the location of a peak associated with a pH reference compound, in relation to a peak associated with a calibration reference compound.

17. The process of claim 16 wherein producing said condition value comprises producing said condition value as a function of said peak location and parameters of a sample solvent.

18. The process of claim 8 further comprising adjusting a set of base reference spectra according to said condition value, to produce said set of reference spectra.

19. The process of claim 18 wherein adjusting said set of base reference spectra comprises adjusting parameters of said base reference spectra according to a pH of the sample.

20. The process of claim 8 further comprising producing a derived reference spectrum in response to said measured condition value and a reference spectrum.

21. The process of claim 20 wherein producing the derived reference spectrum comprises identifying a reference spectrum that is associated with a condition value nearest to said measured condition value.

22. The process of claim 21 wherein producing the derived reference spectrum comprises deriving a value from at least one reference spectrum that is associated with a condition value nearest to said measured condition value.

23. The process of claim 22 wherein producing the derived reference spectrum comprises performing mathematical operations on parameters of a reference spectrum to produce new parameters for use as parameters of said derived reference spectrum.

24. The process of claim 20 further comprising identifying in said test spectrum a peak associated with a calibration compound and producing Lorentzian line shape parameters, including a line width parameter, to represent said peak.

25. The process of claim 24 wherein said derived reference spectrum is represented by at least one set of Lorentzian line shape parameters including a line width parameter, said process further comprising calibrating said line width parameter associated with said derived reference spectrum relative to a line width parameter associated with said calibration compound.

26. The process of claim 25 wherein identifying representative reference spectra comprises adjusting a parameter of said at least one derived reference spectrum until said at least one derived reference spectrum best aligns with said test spectrum.

27. The process of claim 25 wherein identifying representative reference spectra comprises producing a cluster position indicator for a derived reference spectrum,

which causes the positions of peaks in said derived reference spectrum to match corresponding peaks of said test spectrum.

28. The process of claim 25 wherein identifying representative reference spectra comprises producing an upper bound concentration estimate of a quantity of a compound associated with the derived reference spectrum.

29. The process of claim 28 wherein producing an upper bound concentration estimate comprises selecting as said upper bound concentration estimate, a lowest concentration value selected from a plurality of concentration values computed for respective peaks in the test spectrum.

30. The process of claim 29 wherein producing said upper bound concentration estimate comprises finding the height of a peak in the test spectrum that corresponds to a peak in the reference spectrum.

31. The process of claim 30 wherein producing said upper bound concentration estimate comprises determining a concentration value for a peak as a function of said height of said peak.

32. The process of claim 31 producing said upper bound concentration estimate comprises predicting whether said height of a peak in the test spectrum is greater than a threshold level and not determining a concentration for said peak when said height is less than said threshold level.

33. The process of claim 25 further comprising adjusting the relative positions of peaks associated with one of said compounds according to pre-defined criteria.

34. The process of claim 25 wherein identifying representative reference spectra comprises determining scaling factors for peaks in a plurality of reference spectra such that the sum of said peaks scaled by said scaling factors optimally matches said test spectrum.

35. The process of claim 34 further comprising determining concentrations of compounds associated with said reference spectra as a function of said scaling factors.

36. The process of claim 35 further comprising producing an indication of compounds associated with reference spectra having peaks that when scaled by said scaling factors have a height greater than a threshold.

37. The process of claim 35 further comprising outputting a value representing at least one of said concentrations.

38. The process of claim 1 further comprising receiving said test spectrum from a spectrum measurement device.

39. The process of claim 1 further comprising doping the sample with a condition indicator.

40. The process of claim 39 wherein doping comprises doping the sample with a pH indicator.

41. The process of claim 40 further comprising doping the sample with a chemical shift reference compound.

42. The process of claim 41 further comprising employing Nuclear Magnetic Resonance (NMR) to produce free induction decay data operable to be transformed into an NMR spectrum operable to be used as the test spectrum.

43. The process of claim 1 further comprising receiving Nuclear Magnetic Resonance (NMR) free induction decay (FID) data and processing said FID data to produce a representation of a measured spectrum having well defined Lorentzian lines, a flat baseline and peaks that have positive well-defined areas.

44. The process of claim 43 further comprising producing said test spectrum from said measured spectrum.

45. The process of claim 44 wherein producing said test spectrum comprises producing a conditioned spectrum.

46. The process of claim 45 wherein producing said conditioned spectrum comprises producing a baseline corrected spectrum from said measured spectrum.

47. A computer-readable medium for providing computer readable instructions for directing a processor circuit to identify compounds in a sample, the instructions comprising:

a set of codes operable to cause the processor circuit to receive a representation of a measured condition of the sample mixture;

a set of codes operable to cause the processor circuit to use said representation of a measured condition of the sample mixture to select a set of reference spectra of compounds suspected to be contained in said sample mixture, from a library of reference spectra;

a set of codes operable to cause the processor circuit to receive a representation of a test spectrum, produced from the sample mixture under said measured conditions; and

a set of codes operable to cause the processor circuit to combine reference spectra from said set of reference spectra to produce a matching composite spectrum having peaks representing at least some of said suspected compounds, that match peaks said test spectrum, the compounds associated with the reference spectra that combine to produce the matching spectrum being the compound in the sample mixture.

48. A signal embodied in a carrier wave, said signal comprising:

a code segment operable to cause a processor circuit to receive a representation of a measured condition of the sample mixture;

a code segment operable to cause a processor circuit to use said representation of a measured condition of the sample mixture to select a set of reference spectra of compounds suspected to be contained in said sample mixture, from a library of reference spectra;

a code segment operable to cause a processor circuit to receive a representation of a test spectrum, produced from the sample mixture under said measured conditions; and

a code segment operable to cause a processor circuit to combine reference spectra from said set of reference spectra to produce a matching composite spectrum having peaks representing at least some of said suspected compounds, that match peaks said test spectrum, the compounds associated with the reference spectra that combine to produce the matching spectrum being the compound in the sample mixture.

49. An apparatus for identifying compounds in a sample, the apparatus comprising a processor circuit programmed to:

receive a representation of a measured condition of the sample mixture;

use said representation of a measured condition of the sample mixture to select a set of reference spectra of compounds suspected to be contained in said sample mixture, from a library of reference spectra;

receive a representation of a test spectrum, produced from the sample mixture under said measured conditions; and

combine reference spectra from said set of reference spectra to produce a matching composite spectrum having peaks representing at least some of said suspected compounds, that match peaks said test spectrum, the compounds associated with the reference spectra that combine to produce the matching spectrum being the compound in the sample mixture.

50. An apparatus for identifying compounds in a sample, the apparatus comprising:

means for receiving a representation of a measured condition of the sample mixture;

means for using said representation of a measured condition of the sample mixture to select a set of reference spectra of compounds suspected to be contained in said sample mixture, from a library of reference spectra;

means for receiving a representation of a test spectrum, produced from the sample mixture under said measured conditions; and

means for combining reference spectra from said set of reference spectra to produce a matching composite spectrum having peaks representing at least some of said suspected compounds, that match peaks said test spectrum, the compounds associated with the reference spectra that combine to produce the matching spectrum being the compound in the sample mixture.

51. A computer-implemented process for producing a trace file for use in spectrum analysis, the method comprising:

performing a Fourier Transform on Free Induction Decay (FID) data to produce an initial spectrum;

filtering a selected region of said initial spectrum to produce a filtered spectrum; and

phasing said filtered spectrum to produce a measured spectrum having a flat baseline and well defined positive peaks.

52. The method of claim 51 wherein filtering comprises applying a notch filter to said selected region to suppress a peak associated with a contaminant in said contaminant region.

53. The method of claim 52 wherein applying a notch filter comprises producing an adjusted set of notch filter parameters and applying a notch filter employing said adjusted set of notch filter parameters to said selected region.

54. The method of claim 53 wherein applying a notch filter comprises iteratively adjusting said set of notch filter parameters and applying said adjusted notch filter parameters to a notch filter and applying said notch filter to said selected region until a sum of the absolute values of areas defined by peaks above and below a baseline of said initial spectrum is minimized.

55. The method of claim 51 wherein phasing said adjusted spectrum comprises adjusting real and imaginary components of said filtered spectrum until said filtered spectrum has all positive, well defined peaks.

56. The method of claim 51 wherein performing a fourier transform comprises performing a weighted Fourier Transform with weights that provide for enhancement of said initial spectrum.

57. The method of claim 56 wherein performing a weighted Fourier Transform comprises employing weights that perform a line broadening function to said initial spectrum.

58. The method of claim 51 further comprising defining the size of a window on said initial spectrum.

59. The method of claim 58 wherein defining the size of a window comprises scaling said initial spectrum.

60. The method of claim 51 further comprising correcting said initial spectrum for drift effects.

61. The method of claim 51 further comprising performing baseline correction on said measured spectrum.

62. A computer readable medium for providing codes operable to direct a processor circuit to produce a trace file for use in spectrum analysis, the computer readable medium comprising:

codes for automatically causing the processor circuit to perform a Fourier Transform on Free Induction Decay (FID) data to produce an initial spectrum;

codes for automatically causing the processor circuit to filter a selected region of said initial spectrum to produce a filtered spectrum; and

codes for automatically causing the processor circuit to phase said filtered spectrum to produce a measured spectrum having a flat baseline and well defined positive peaks.

63. An apparatus for producing a trace file for use in spectrum analysis, the apparatus comprising:

means for automatically performing a Fourier Transform on Free Induction Decay (FID) data to produce an initial spectrum;

means for automatically filtering a selected region of said initial spectrum to produce a filtered spectrum; and

means for automatically phasing said filtered spectrum to produce a measured spectrum having a flat baseline and well defined positive peaks.

64. A signal for causing a processor circuit to produce a trace file for use in spectrum analysis, the signal including:

a first segment comprising codes for automatically causing said processor circuit to perform a Fourier Transform on Free Induction Decay (FID) data to produce an initial spectrum;

a second segment comprising codes for automatically causing the processor circuit to filter a selected region of said initial spectrum to produce a filtered spectrum; and

a third segment comprising codes for automatically causing the processor circuit to phase said filtered spectrum to produce a measured spectrum having a flat baseline and well defined positive peaks.

65. A computer-implemented process for producing a representation of a spectrum for a hypothetical solution containing a compound, for use in determining the composition of a test sample, the process comprising:

producing a position value for at least one peak of a reference spectrum as a function of a measured condition of the test sample, and a property of said at least one peak in a base reference spectrum

66. The process of claim 65 wherein producing a position value comprises interpolating said position value from position values associated with base reference spectra associated with a condition nearest to said measured condition.

67. The process of claim 65 wherein producing a position value comprises calculating said position value as a function of pH of said sample.

68. The process of claim 65 wherein producing a position value comprises producing said position value by addressing a lookup table of position values with a measured condition value representing said condition of said sample.

69. The process of claim 65 further comprising accessing a pre-defined record specifying peaks in a reference spectrum and adjusting a position value in said record, said position value being said position value of said at least one peak.

70. The process of claim 69 wherein adjusting comprises locating a condition value dependent function in said pre-defined record, producing said position value from said function and associating said position value with said pre-defined record.

71. The process of claim 70 wherein associating comprises storing said position value in said pre-defined record.

72. The process of claim 69 wherein adjusting comprises locating in said pre-defined record a link to a lookup table specifying peak positions for various conditions and retrieving said position value from said lookup table and associating said position value with said pre-defined record.

73. The process of claim 72 wherein associating comprises storing said position value in said pre-defined record.

74. A computer-readable medium for providing computer readable instructions for causing a processor circuit to produce a representation of a spectrum for a hypothetical solution containing a compound, for use in determining the composition of a test sample, the instructions comprising:

a set of codes for directing the processor circuit to produce a position value for at least one peak of a reference spectrum as a function of a measured condition of the test sample, and a property of said at least one peak in a base reference spectrum.

75. A signal operable to cause a processor circuit to produce a representation of a spectrum for a hypothetical solution containing a compound, for use in determining the composition of a test sample, the signal comprising a signal segment comprising codes operable to cause the processor circuit to produce a position value for at least one peak of a reference spectrum as a function of a measured condition of the test sample, and a property of said at least one peak in a base reference spectrum.

76. An apparatus for producing a representation of a spectrum for a hypothetical solution containing a compound, for use in determining the composition of a test sample, the apparatus comprising a processor circuit programmed to produce a position value for at least one peak of a reference spectrum as a function of a measured condition of the test sample, and a property of said at least one peak in a base reference spectrum.

77. An apparatus for producing a representation of a spectrum for a hypothetical solution containing a compound, for use in determining the composition of a test sample, the apparatus comprising:

means for receiving a measured condition value representing a condition of the test sample;

means for receiving a representation of a position of at least one peak in a base reference spectrum; and

means for producing a position value for at least one peak of a derived reference spectrum as a function of said measured condition value of the test sample, and the position of said at least one peak in a base reference spectrum.